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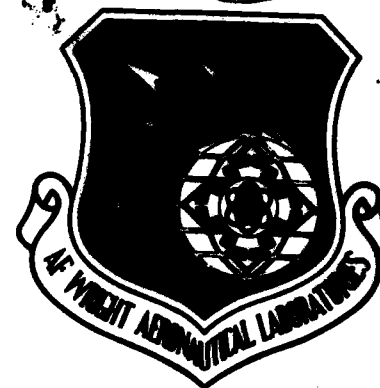
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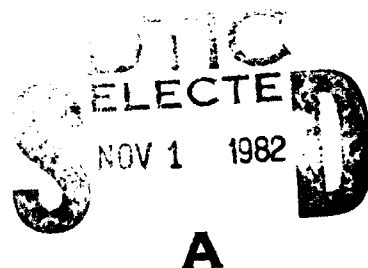
COMPOSITIONAL, ATOMIC AND MOLECULAR ANALYSIS IN SUPPORT
OF MATERIALS NEEDS OF THE U.S. AIR FORCE

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September 1982

Final Report for Period May 1980 - May 1982

Approved for public release: distribution unlimited.



MATERIALS LABORATORY
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AIR FORCE SYSTEMS COMMAND
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This technical report has been reviewed and is approved for publication.

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20. Major areas of effort include atomic spectroscopy, microanalysis, mass spectrometry and molecular spectroscopy. A brief discussion of the effort in each of these areas is given along with the number of samples analyzed by various techniques during the period of contract performances.

FOREWORD

This report was prepared by the Department of Chemistry, Miami University, Oxford, Ohio under Air Force Project No. 241807, "Systems Support," Task No. 2418, "Aerospace Structural Materials." The work was administered under the direction of the Materials Laboratory, Air Force Systems Command, Wright-Patterson Air Force Base, Ohio, Contract #33615-80-C-5002. Mr. James Muntz (AFWAL/MLU) served as Project Engineer.

The work was performed at Miami University and at the Materials Laboratory, Wright-Patterson AFB during the period 12 May 1980 through 15 May 1982. The report was submitted by the author in June 1982.

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SECTION I

INTRODUCTION

This report was prepared by the Department of Chemistry, Miami University, Oxford, Ohio and is the final report of USAF Contract F33615-80-C-5002. It covers the period 12 May 1980 - 15 May 1982. The work was performed at Miami University and at the Materials Laboratory, Wright-Patterson Air Force Base, Ohio. The major participants were Messrs. J. R. Kerns, T. E. Kerschner and T. H. Stout, Mrs. Anne Papania and Drs. Chi K. Yu and J. E. Katon. Dr. J. E. Katon served as Project Leader. The contract involved method development, support programs, service functions, materials characterization and development and application of analytical techniques of various kinds in support of Air Force programs. It also involved research in the areas of molecular structure determination and materials characterization.

The rapid development of aerospace science in the last thirty years has resulted in the synthesis and development of many new materials possessing unusual chemical and physical properties. This rapid development of new and exotic materials has required that a good deal of effort be expended in the development of new techniques to analyze and characterize them. Seldom are the classical methods applicable to these new compounds and therefore a good deal of research and method modification is necessary to develop new techniques. Once such techniques are developed, they must be applied to the analysis of such new experimental methods.

In addition to the analysis and characterization of experimental materials, the need often arises for accurate and expeditious analysis of samples arising from practical problems encountered by the Air Force in one of its many widespread areas of operation. This is most generally typified by accident investigations or equipment malfunctions.

Because of the sometimes rapidly changing requirements of the Air Force, the effort on the contract has varied at times with regard to the particular areas of emphasis. For instance, efforts in atomic spectroscopy, X-ray diffraction and separations have varied widely over the course of the contract. Some months these areas have required nearly a full man-month while other months have required little effort. The effort in infrared spectroscopy has been relatively constant over the contract period as has mass spectrometry, but the purchase of the Finnigan 4021 system has led to more efficient sample handling at the end of the contract. Microanalysis required an essentially constant level of effort. During the past two years there has been a great increase in the number of "problem-solving" samples. These samples require new techniques or the combination of two or more techniques if the desired characterization is to be obtained. Such samples are both challenging and time-consuming, but are, in general, very important to the mission of the Air Force.

A significant amount of the service work has been subcontracted to other organizations during the performance of this work. This involves primarily specialized service and support functions which can be provided by organizations which have particular capabilities in the required fields. The rate of subcontracted effort decreased drastically as the contract effort progressed, however, due to the development of in-house capabilities to perform these specialized functions when there existed a continuing need. In-house performance of these functions is desirable since it results in a large time-saving, in general.

The succeeding sections of this report summarize the effort expended and the results obtained in the various areas during the performance of contract F33615-80-C-5002

SECTION II

MICROANALYSIS

A relatively large effort in microanalysis was required throughout the contract period on a continuing bases. The largest number of samples received for analysis were those requiring microanalytical procedures of some type.

Within the area of microanalysis, carbon and hydrogen determinations are by far the most requested single analysis. These are normally performed on the Perkin-Elmer Model 240 C,H,N analyzer. This instrument is now rather old and is obsolete in the sense that newer models require considerably less operator time per analysis. During the period of the contract rather severe downtime problems were encountered from time to time. Each of these was corrected, but such behavior is expected to continue and perhaps increase due to the age of the instrument. During instrument downtime periods the C, H analyses must be run by the Pregl method. This is considerably more time consuming. In addition this method is not suitable for nitrogen determination.

Included in the microanalysis area are many other quantitative determinations of other elements present in samples as well as certain physical properties. Also included are molecular weight determinations by vapor pressure osmometry.

Occasionally, microanalyses are subcontracted. These are usually because the sample submitter requests that the work be done by a particular laboratory since they are particularly qualified or because of particular time constraints with individual samples.

The number of microanalyses of various kinds performed during this contract are summarized below.

Type of Analysis	Determinations	
	In-house	Subcontracted
1. Carbon and Hydrogen	728	7
2. Nitrogen	378	5
3. Chlorine	144	1
4. Bromine	141	0
5. Iodine	57	0
6. Oxygen	0	23
7. Sulfur	180	0

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Type of Analysis		Determinations	
No.	Description	No.	Description
1	...	1	...
2	...	2	...
3	...	3	...
4	...	4	...
5	...	5	...
6	...	6	...
7	...	7	...
8	...	8	...
9	...	9	...
10	...	10	...

SECTION III

MASS SPECTROMETRY

There is a continuous demand for mass spectrometric analyses. Often the demand extends to separations and thus leads to a need for gas chromatographic-mass spectrometric analyses. Such samples may require the actual analysis of many components of a given sample. As a result, one sample may require as much as a man week of effort. During the period of this contract there was a continuous need for one-man per year total effort and occasionally a need for further effort.

Basically, effort was spent on three instrument systems. The DuPont 21-490 Chemical Ionization Mass Spectrometer was the major instrument used during the first fifteen months of the contract period. In August 1981 the new Finnegan 4021 GC/MS/DS system became operable and the majority of samples received were analyzed with this new system. It should be noted that the DuPont 21-490 was maintained in operation, however, as it is the only system capable of analyzing materials with molecular weights over 1000. Both instruments were therefore kept in operation. During the contract a continuous effort, on a "as time is available" basis, was spent to put into operation the CEC 110-B High Resolution Mass Spectrometer. This was finally accomplished in March, 1982.

Samples analyzed during the period of this contract were as listed:

GC/MS	358
MS only	<u>468</u>
Total	826

SECTION IV

MOLECULAR SPECTROSCOPY

The effort in the area of molecular spectroscopy over the period of this contract was exclusively limited to infrared spectroscopy. There was, however, a wider than usual requirement for unusual procedures and equipment. A great deal of difficulty was encountered with the infrared spectrometers located at WPAFB (Perkin-Elmer Models 521 and 621) and a large amount of instrument downtime was experienced. At the very end of the contract a new Perkin-Elmer Model 683 Infrared Spectrophotometer was purchased by the Air Force and this instrument should make service in this area much better in the future. The availability of special equipment at Miami University led to a relatively large number of samples being analyzed there. These involved special requirements and equipment not available at WPAFB.

The total number of service samples analyzed during the contract period was 577 at WPAFB and 158 at Miami University. It should be noted that many of these samples require the recording of several spectra for complete analysis. This has been particularly evident in the field over this contract period as more and more difficult samples and problems have been encountered. This is particularly true of samples analyzed at Miami University, but is also true of the samples analyzed at WPAFB. Of the samples analyzed at Miami University, 18 required Fourier Transform Infrared Spectroscopy, 49 required Computer Assisted Dispersive Infrared Spectroscopy, 75 required the high resolution, high precision and accuracy afforded by a research instrument (PE Model 180), 6 required far infrared spectroscopy, 6 required low temperature infrared spectroscopy, and 4 required quantitative analysis for p-dibromobenzene. The last was done by developing an infrared spectroscopic method at Miami University prior to analyzing the samples. It utilizes the 810 cm^{-1} band of p-dibromobenzene and the Beer's Law plot has good linearity over the concentration range 2×10^{-3} - 9×10^{-3} molar. Average error within these limits is about 4%.

As a part of a study of the spectra and structures of biologically important small molecules, the pyruvate series of molecules have been studied. This study consisted of a series of detailed studies on selected molecules and a survey of the carbonyl stretching frequencies of a number of other molecules. The studies can be summarized as:

- 1) Pyruvoyl Chloride - This compound is thermally unstable and therefore all sample-handling and data-gathering was carried out at -20°C or below. The compound was synthesized by a previously reported procedure. As an

aid to the assignment, pyruvoyl bromide, which does not appear to have been previously reported, was synthesized and its infrared spectra recorded. The spectra indicate that pyruvoyl chloride has a structure similar to that of other pyruvic acid derivatives in the crystal. It is planar, or near planar, with the two carbonyl groups trans to one another.

2) Pyruvic Acid - The vibrational spectra of pyruvic acid have been obtained, analyzed and assigned. These spectra have allowed conclusions concerning the structure and the nature of the hydrogen bonding present to be obtained under various conditions. In the pure solid and liquid phases pyruvic acid exists as a cyclic, hydrogen-bonded dimer in which the keto oxygen is not involved in hydrogen bonding. In the liquid phase, this structure is in equilibrium with a significant amount of enol structure. In dilute solution, the structure is that of an internally hydrogen-bonded monomer in which the keto group is involved in the hydrogen bond but the acid carbonyl is not.

3) 3-Bromopyruvic Acid - The spectra and structure of 3-bromopyruvic acid were investigated and compared to those of pyruvic acid. It has been found that the spectra of 3-bromopyruvic acid in the liquid phase and in solution are very similar to those of pyruvic acid indicating similar structures (cyclic dimer in the liquid phase, cyclic monomer in dilute solution). The solid state spectra are quite different, however. The solid state spectra of 3-bromopyruvic acid show a center of symmetry, but the OH stretch is that of an alcohol, not an acid. Only one carbonyl functionality is observed and there is no olefinic carbon-carbon stretching mode.

The spectra have been analyzed and interpreted in terms of a cyclic hydroxylactone structure which can arise by the addition of the acid OH of one molecule across the keto carbon-oxygen double bond of a second molecule. This forms an unusual dimer structure which is really a condensation dimer rather than the usual hydrogen-bonded dimer formed by acids. The condensation is a reversible reaction, however - the normal structure being formed when the crystal melts.

4) Carbonyl Stretching Bands of Pyruvate Molecules - The infrared and Raman spectra in the carbonyl stretching region have been recorded for a number of molecules of the pyruvate series. This data has been compared with previously published data for the oxalate series. Analysis of these spectra indicates that there is little or no electronic interaction between the two unsaturated centers. It is therefore concluded that each carbonyl stretching mode in the infrared spectra of the pyruvate series reflects its own particular functionality.

In addition, two further studies of particular molecules of interest, were completed. A study of the vibrational spectra and structures of cyclobutanecarbonyl chloride in various phases has been completed. This study required the synthesis of cyclobutanecarbonyl bromide and the α -deuterated derivatives of both molecules. It was shown that the two halides exist as a conformational equilibrium mixture in the gaseous and

liquid states but not in the solid state. The two conformers have very similar spectra, however. In view of this it appears likely that the conformational change is one in which the substituent changes from the axial to the equatorial conformation, not the one in which the COCl group rotates about the ring-substituent bond. Although the second conformational change is possible, and probably does occur to some extent, its energetics appear to be such that only a very small amount of one conformer exists. A complete vibrational assignment of the four compounds was carried out.

High resolution infrared spectra of oriented polycrystalline films of m-dinitrobenzene have been recorded at about 20K using polarized radiation. The spectra have been completely interpreted and the intermolecular coupling within the unit cell has been observed and is consistent with the previously reported crystal structure (X-ray diffraction). The relative intensities of the observed factor group components have been used to determine the symmetry species of the corresponding molecular transitions, leading to an improved vibrational assignment. There is evidence that considerable intramolecular motion remains even at low temperature. This motion appears to be associated with a torsional motion of the NO₂ groups about the CN bond.

SECTION V

ATOMIC SPECTROSCOPY

Significant effort in the area of atomic spectroscopy was expected on this contract due to experience with the preceding contract. The actual requirements in this area were sporadic, however. During certain busy months a significant effort was required for both service analyses and method development. However, some months did not experience any requests. Major projects included the analysis of eight samples for 10 elements, each in the part per billion range, the attempt to develop an atomic absorption method for the analysis of palladium (a satisfactory method was not developed using AA, but a colorimetric method was), and the development of a new sample digestion method which led to a very satisfactory atomic absorption analysis method for nickel in certain samples.

The breakdown of analyses of a service nature for the contract period is as follows: Ag - 199, Sn - 20, Ni - 16, Al - 15, Y - 5, K - 5, Sb - 5, Pb - 3, Li - 3, Mn - 2, Zn - 1, Ca - 1, Ba - 1, Na - 1. Total elemental analyses by AA - 357

SECTION VI

SEPARATIONS

Separations became an area of rather wide demand during the period of the contract, but was limited to two methods in terms of this report (gas chromatography was routinely done in conjunction with mass spectrometry, see Section III). These two methods are high performance liquid chromatography (HPLC) and gel permeation chromatography (GPC). A fair amount of time was spent in developing methods for particular samples during the time of this contract, only a few samples being routine, at least initially.

Sixteen samples were received for molecular size and molecular weight comparisons. A GPC procedure to determine the desired information for these polymeric materials was developed. Gradient elution HPLC methods for four samples consisting of mixtures of structural isomers were also developed. Four samples of diaminodiphenylsulfones in graphite epoxy were received for HPLC and required the development of a reverse phase procedure. Two samples of dye mixtures were received and separated. These were extremely complex mixtures. Many of the samples received, both routine and non-routine, required extra care in separation and collection of fractions which were then further analyzed by infrared or mass spectrometric methods. Other routine samples consisted of 22 samples for HPLC and 26 samples for GPC.

SECTION VII

POWDER X-RAY DIFFRACTION ANALYSES

Work in this area during the contract period was almost exclusively routine. A large number of samples of construction samples were received for identification as asbestos or not. If these materials are asbestos, the type of asbestos is often required. Other samples are widely variable - corrosion products, residues, miscellaneous crystalline unknowns from accident investigations, etc. The number of samples received were: asbestos - 70, miscellaneous - 82. Total samples analyzed by X-ray diffraction = 152.

SECTION VIII

GENERAL ANALYTICAL SUPPORT

1. Routine analyses

Carbon in Steel	-	134
Sulfur in Steel	-	38
Analytical Weighings	-	32
Isocyanate analyses	-	16
Iron analyses	-	16
(titration)		
Water Hardness	-	6
Density	-	6
Nickel analyses	-	7
(gravimetric)		
Nitrate analyses	-	7
Carbon in TiC	-	4
Chlorine in metals	-	3
Silicon in metals	-	2
Conductivity	-	2
Soxhlet Extractions	-	2
Sucrose analyses	-	2
Freezing Point	-	1
Brine (specification	-	3
analysis)		
Mercury analysis	-	1
Vanadium analysis	-	1
Yttrium	-	26
CaCO ₃	-	4
Water solubility	-	4
Moisture content	-	4
		—
Total routine analyses -		321

2. Non-Routine Effort

During the contract period a significant amount of effort was expended in "solving problems". These involve an extremely wide variety of samples ranging from accident investigation samples to manufactured products which are not meeting specifications. Many times a variety of analytical procedures must be used to answer the questions of the sample submitter. These may be single procedures or a combination of several. In addition, new methods may need to be developed to perform the analyses requested. As an example, the development of a method to determine the amount of oxirane functional group in Epoxies may be cited. This method was then applied to eight samples. There are many other specific examples, but since they are unrelated, a listing does not appear appropriate in a summary report. In addition, many are involved in accident or failure cases and the information is not approved for public dissemination in terms of this report.

SECTION IX

SUBCONTRACTED ANALYSES

A number of analyses are routinely subcontracted to various laboratories. This arises because (1) these laboratories are particularly skilled in the analysis; (2) they have specialized expensive equipment necessary for the analysis; (3) the number of analyses of this kind do not justify setting up in-house procedures; or (4) the in-house equipment is undergoing maintenance or repairs and it is important that results be obtained quickly. A summary of the analyses subcontracted during this contract is given below. This does not include microchemical analyses subcontracted (See Section II).

1. Nonmetallic Elemental Analyses

Sample Type	C	H	O	N	Cl
1. Titanium	101	95	123	95	16
2. Aluminum	2	12	30	6	-
3. Titanium Alloys	56	59	60	56	2
4. Aluminum Alloys	3	2	6	1	-
5. Titanium/Aluminum	7	11	13	7	-
6. Fe ₃ Si	2	2	3	2	-
7. SiC/AlN	-	-	18	-	-
8. Si ₃ N ₄	-	-	5	5	-
9. TiC	3	-	6	-	-
10. Al/Fe	2	10	2	-	-
11. Fe/Al	2	-	3	2	-
12. Steel	-	-	-	8	-
13. Ni/Cu	-	-	7	-	-
14. Ni/Al	4	-	4	-	-
15. Ni/Co	-	-	8	-	-
16. Nickel	4	-	-	-	-
17. Miscellaneous Alloys	<u>5</u>	<u>2</u>	<u>2</u>	<u>2</u>	<u>-</u>
TOTALS	191	193	290	184	18

Total Nonmetallic Elemental Analyses - 876

II. Metallic Elemental Analyses and Chemical Analyses

Sample Type	Analysis
1. Alloys	Ni - 48, Mo - 29, Al - 70, Fe - 33, W - 15, Zn - 3, Si - 4, Cu - 8, Zr - 3, V - 3, Chem. Anal - 3. TOTAL = 219
2. Metals	Chem. anal - 2, Emission spectrographic analysis - 8. TOTAL 10.
3. Powder	Chem. anal - 1
4. Silver	Assays - 4
5. Mallite	Al - 2, Si - 2. TOTAL = 4
6. Yttrium	Y - 75

Total Metallic Elemental Analyses and Chemical Analyses = 313

III. Miscellaneous Analyses

1. PCB - 17
2. Surface area - 9
3. Spark source mass spectrometric analyses - 22
4. GC/MS analyses - 26
5. Nuclear Magnetic Resonance Spectral Analyses - 53
6. Residual Gas Analyses - 5
7. Solid Waste Analyses - 2
8. Arsenic in Oil Shale - 2
9. Dust Identification - 3

Total Miscellaneous Analyses = 139

Total Subcontracted Analyses = 1328

BIBLIOGRAPHY

During the time period covered by this report the following papers, articles and reports based in whole, or in part, on work performed under this contract were published. In most cases, a significant portion of the work was also supported by Miami University. The coauthors of the various publications were/are students at Miami University according to the following.

G. N. R. Tripathi, Postdoctoral Research Associate, 1977-8
W. J. Ray, Ph.D., Miami University, 1980
K. Hanai, Postdoctoral Research Associate, 1978-9
P. H. Chu, M.S., Miami University, 1980
R. D. Moore, Ph.D., Miami University, 1978
S. R. Lobo, Ph.D. student, Miami University, 1979-
J. M. Landry, Ph.D. student, Miami University, 1979-

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Its Derivatives", Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy, Atlantic City, New Jersey, 1980.

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